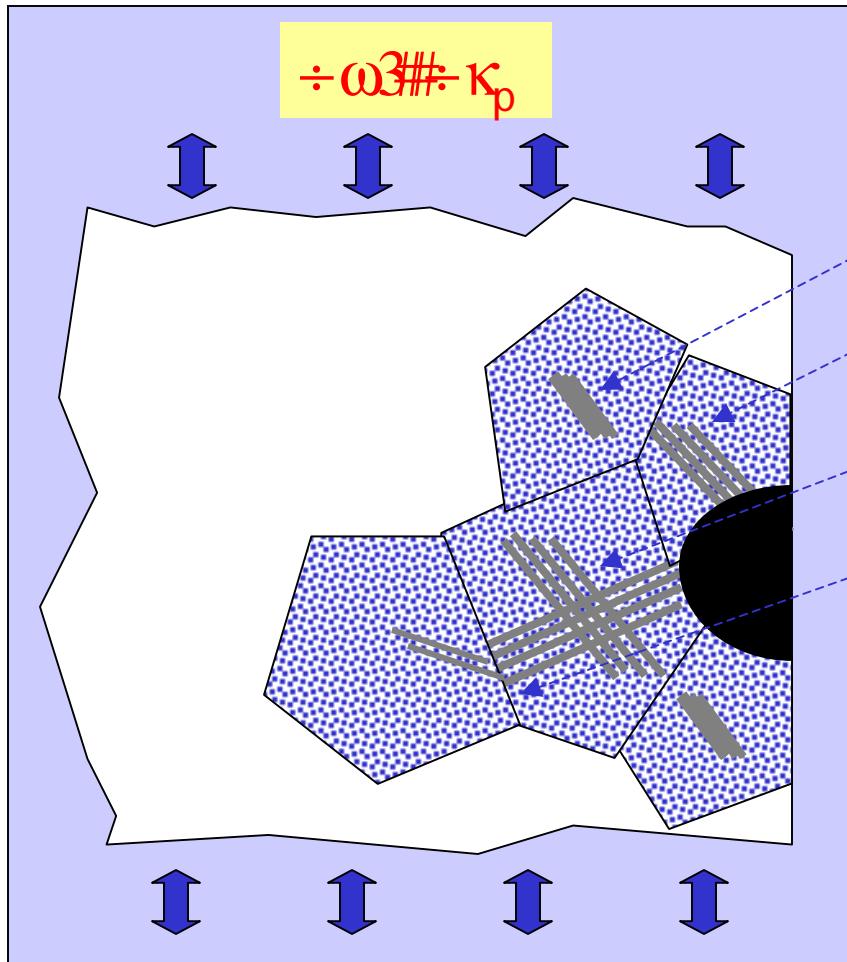


VISION : Predict Microstructure-Sensitive Cyclic $\omega 4\kappa$ Curves !



σ4structure Sensitivity of Plasticity in MONOTONIC Loading

Slip Initiation : Source Strengths

Dislocation-Precipitate Interactions

Multislip Work-Hardening within Grain

Grain-Grain Interaction

Bridge with
FATIGUE MODELS
(McDowell, ..)

Cyclic Slip, Slip Localization

Key : Include as many Microstructural & Chemistry Variables as Possible

OUTLINE

Microstructure Effects Within Grains ($v_2 v'$)

Using DD SIMULATIONS (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

- PROGRESS : Established a Working Model / Methodology
- CURRENT FOCUS : Connectivity ("Handshakes")

Using FEM (Y-S Choi, T.A.Parthasarathy, D.M.Dimiduk)

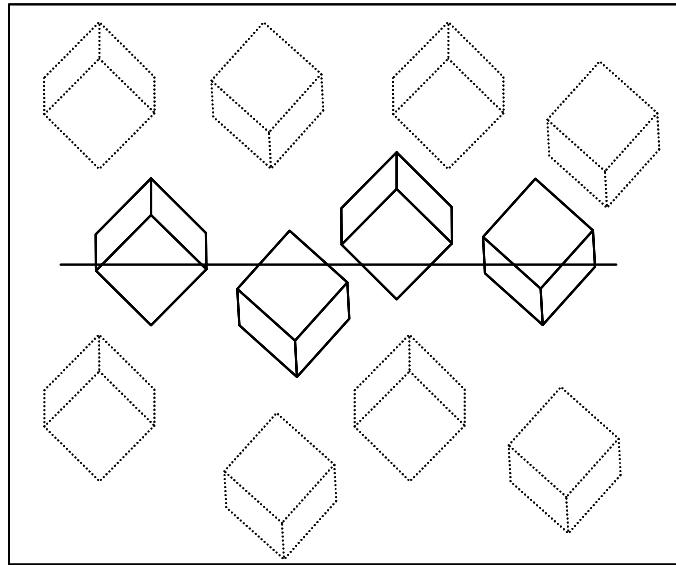
- Unit Cell Model : Identified Key Issues - Refinements

Grain-Grain Interaction

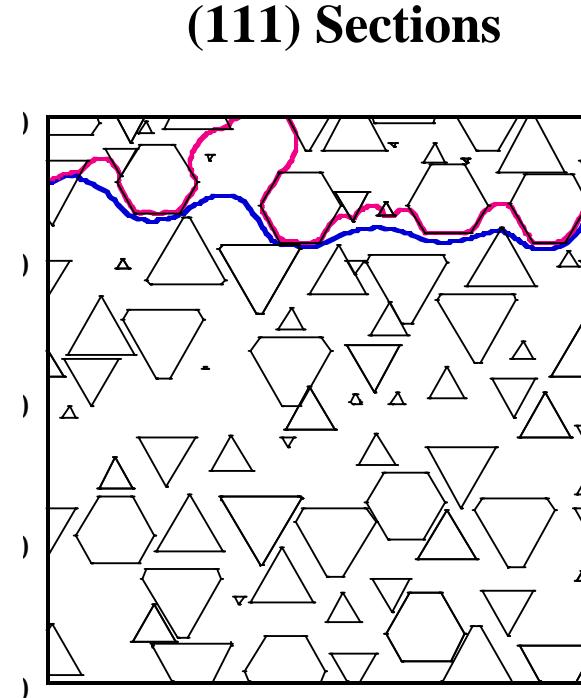
- Polycrystal Model : Using DD results

Grain-Defect Interaction

Discrete Dislocation (DD) Simulations



*Random Distribution
of Cubes in a box*



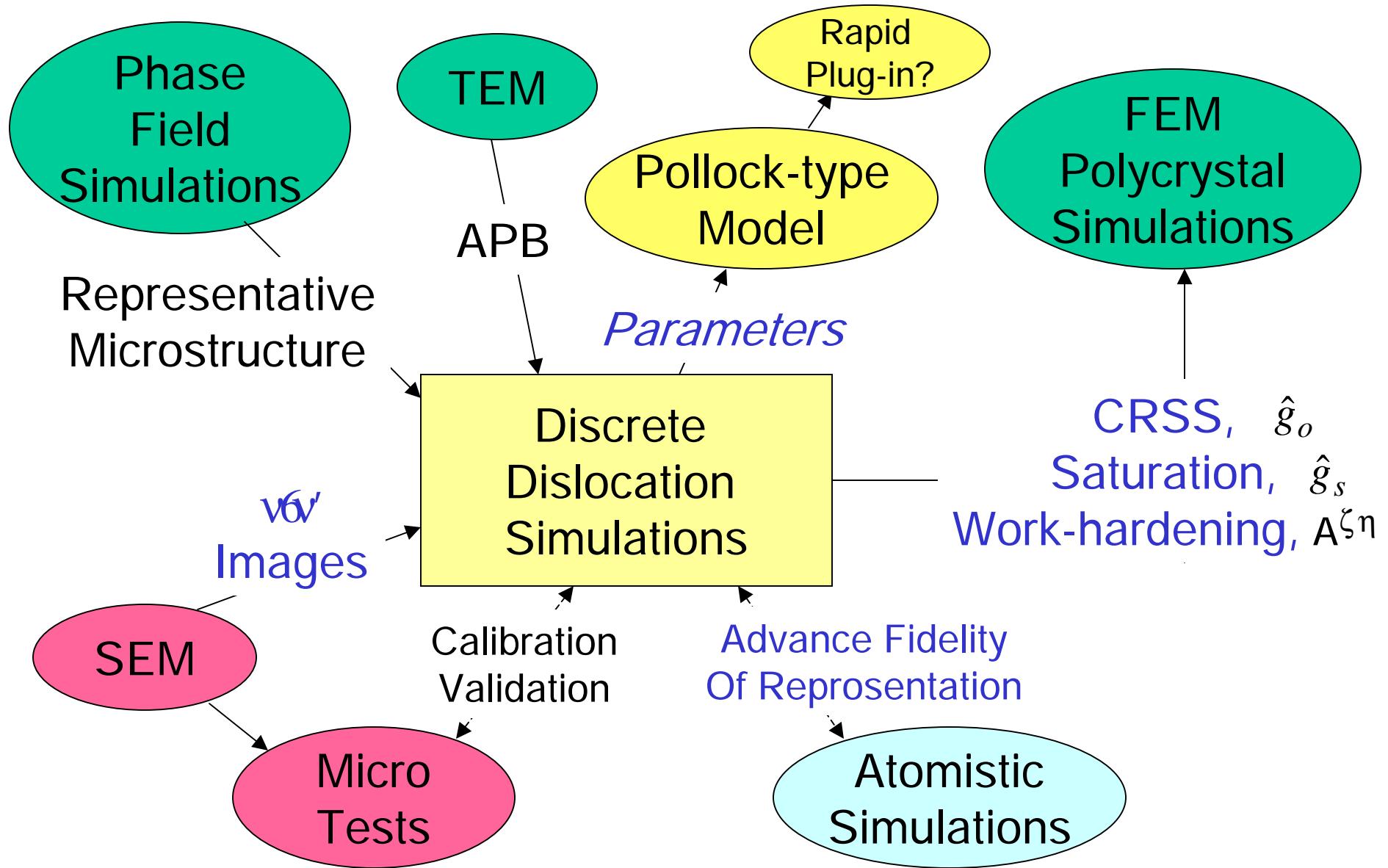
*Spatial Distribution
Varies with Plane of Sectioning*

DD : Established 2D Methodology (Low T athermal)

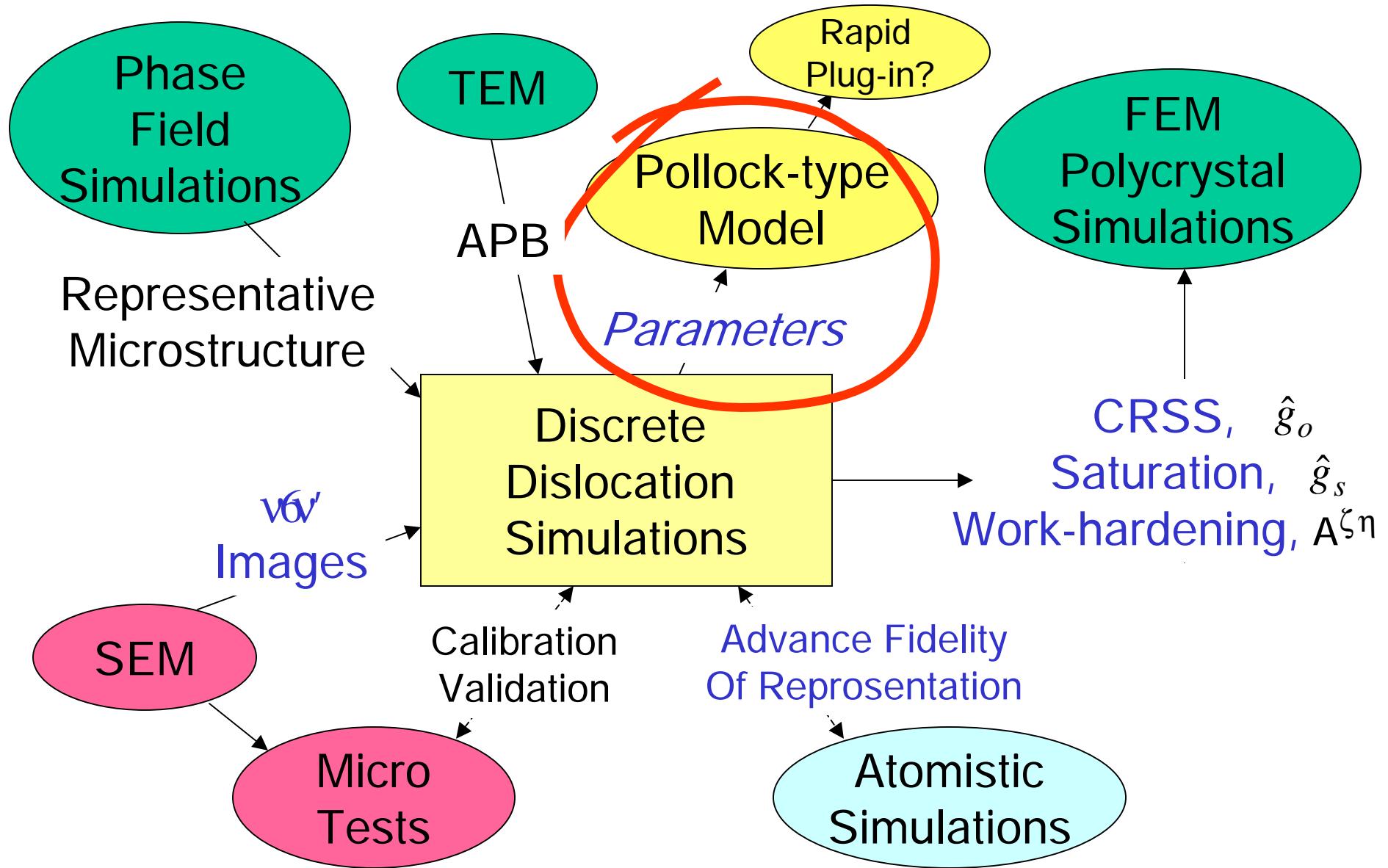
<u>Model</u>	<u>Findings : Parametric Studies</u>	<u>Issues</u>
Precipitate Hardening	Differs from Analytical Model (Reppich) Size & V_f Dep. Reasonable (Expt.) Real Microstructure Simulated	Other Models ? Scatter, ~10% Thresholding
	APB Energy : Primary Factor Friction Stress in v Significant Coherency, Curvature : Negligible	Measure/Calc. Measure ?
Multi-Slip WH	3D with cross-slip (Comp. Limited)	Parallel Proc. (CHSSI, AFOSR)

Need "Handshakes" to Meet AIM Goals

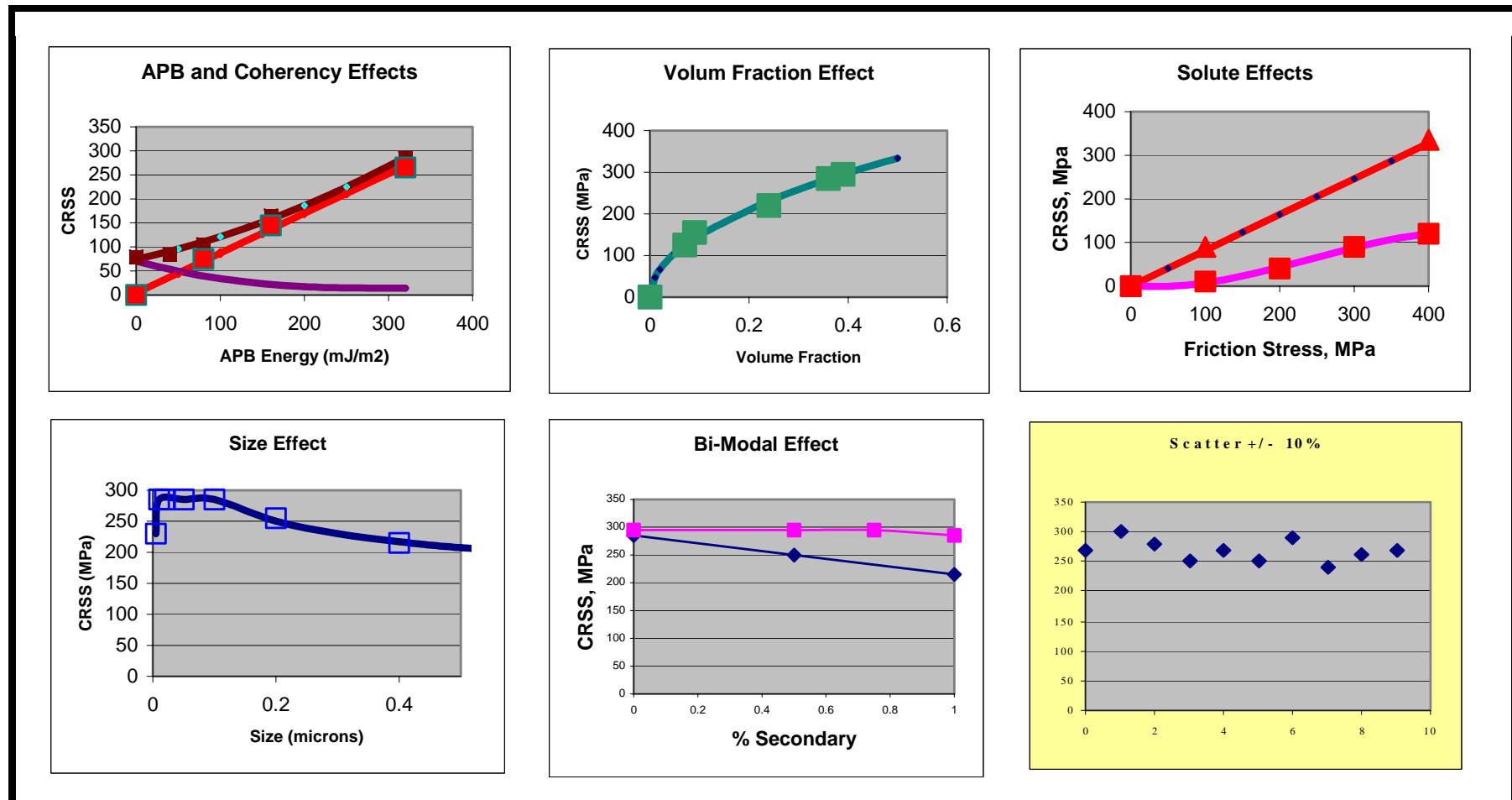
DD : Current Focus - Connectivity ("Handshakes")



DD : Current Focus - Connectivity ("Handshakes")



DD Parametric Studies



Fits to Parametric Studies => Pollock-type Model

Pollock-type Model : (derived from DD results)

CRSS =

APB

Min Ψ

$$\left(A_1 \cdot 2 \cdot A_2 \cdot B_{APB} \right) \cdot 2$$

Coherency

Volume Fraction

$$2 \left(C_1 \cdot 4 \cdot C_2 \cdot B_{APB} \cdot 2 \cdot C_3 \cdot B_{APB}^2 \cdot 4 \cdot C_4 \cdot B_{APB}^3 \right) \frac{C}{0.3} \cdot qV_f^{0.5} \epsilon,$$

$$, \left[S_1 \cdot \Psi_a / V_f^{40.5} \cdot 410 \cdot \beta^{4S_2} \right]$$

Ppt Size

+

F''

$$\left[P_1 \cdot 2 \cdot P_2 \cdot \vartheta_v \cdot 2 \cdot P_3 \cdot \vartheta_v^2 \right],$$

$$\left[M_1 \cdot \vartheta_v^{M2} \right] \epsilon$$

Ppt Sol. Str.

Matrix Sol. Str.

$$\omega_Y + (14 f_{v'})'' (M(CRSS) \cdot 2 k_{v2v'} d_{v2v'}^{40.5}) \otimes f_{v'} / \vartheta_{0v'} \cdot 2 k_{v'} d_{v'}^{40.5} ($$

IN 100 - Spreadsheet

Data from Pollock's slides

Clement / Nembach

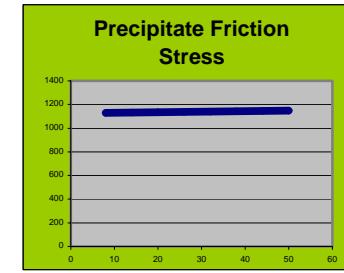
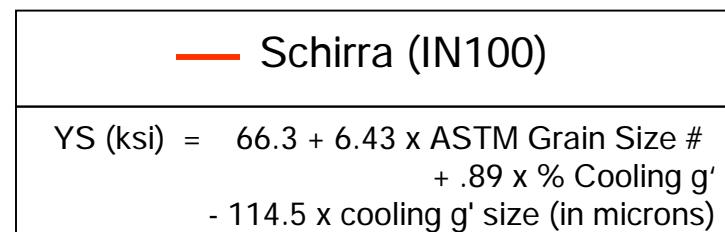
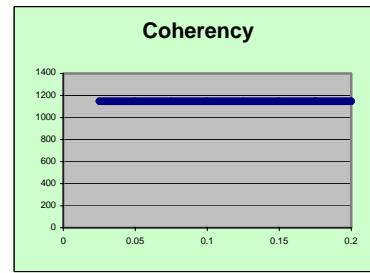
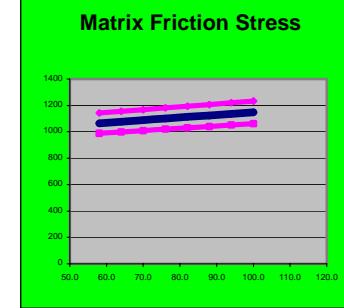
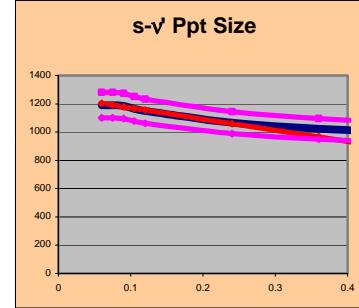
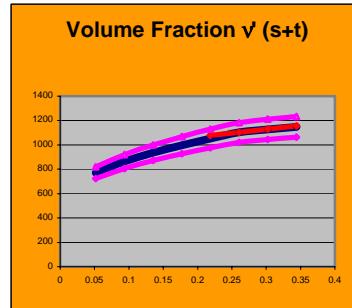
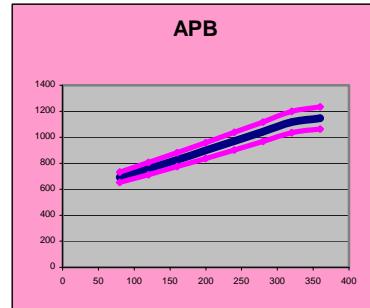
Exp.

Coh %	Vf-Total	Vf-t	Size-t	Vf-s	Size-s	Vf-p	Size-p	d _(v2v)	sol-g	sol-g'
0.1 0.0125	0.544	0.01	0.006	0.334 0.04175	0.12 0.015	0.2	1.7	3.82	100 6	50 6

*Fit
Par.*

APB	M	k _v
360 40.00	3	500

k _{v-Pv}
500



Data from Pollock on IN100 (PWA 1100 - ver.3)

Data from Pollock's slides

Exp.

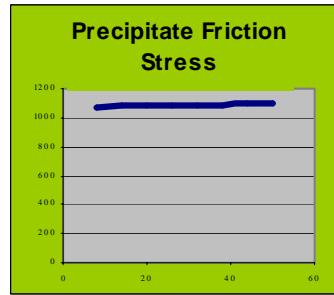
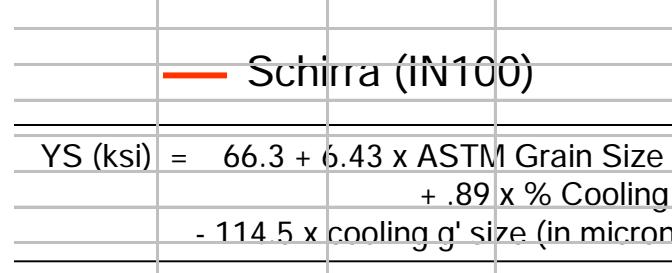
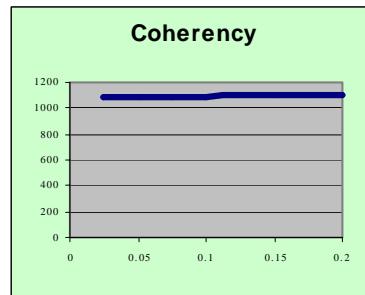
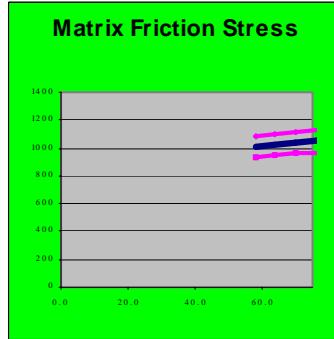
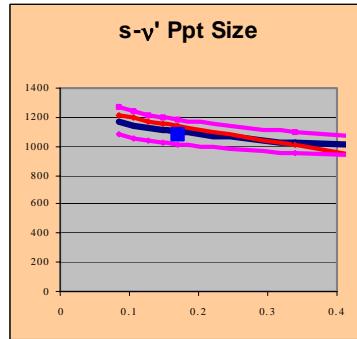
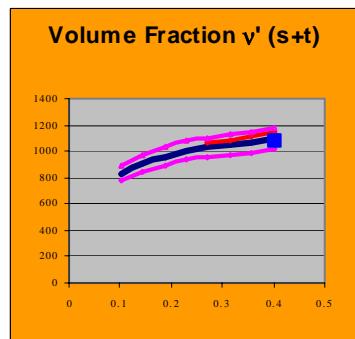
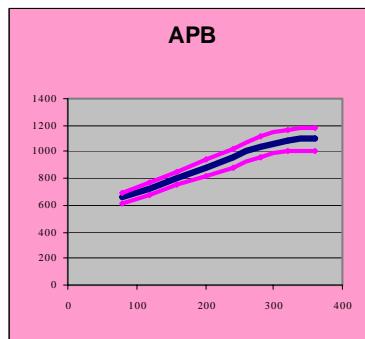


oh %	Vf-Total	Vf-t	Size-t	Vf-s	Size-s	Vf-p	Size-p	$d_{(v2v')}$	sol-g	sol-g'
0.1	0.6	0.06	0.002	0.34	0.17	0.2	1.2	4.1	100	50
0.0125				0.0425	0.02125				6	6

*Fit
Par.*

APB	M	k_v
360	3	450
40.00		

$k_{v'-Py}$
450

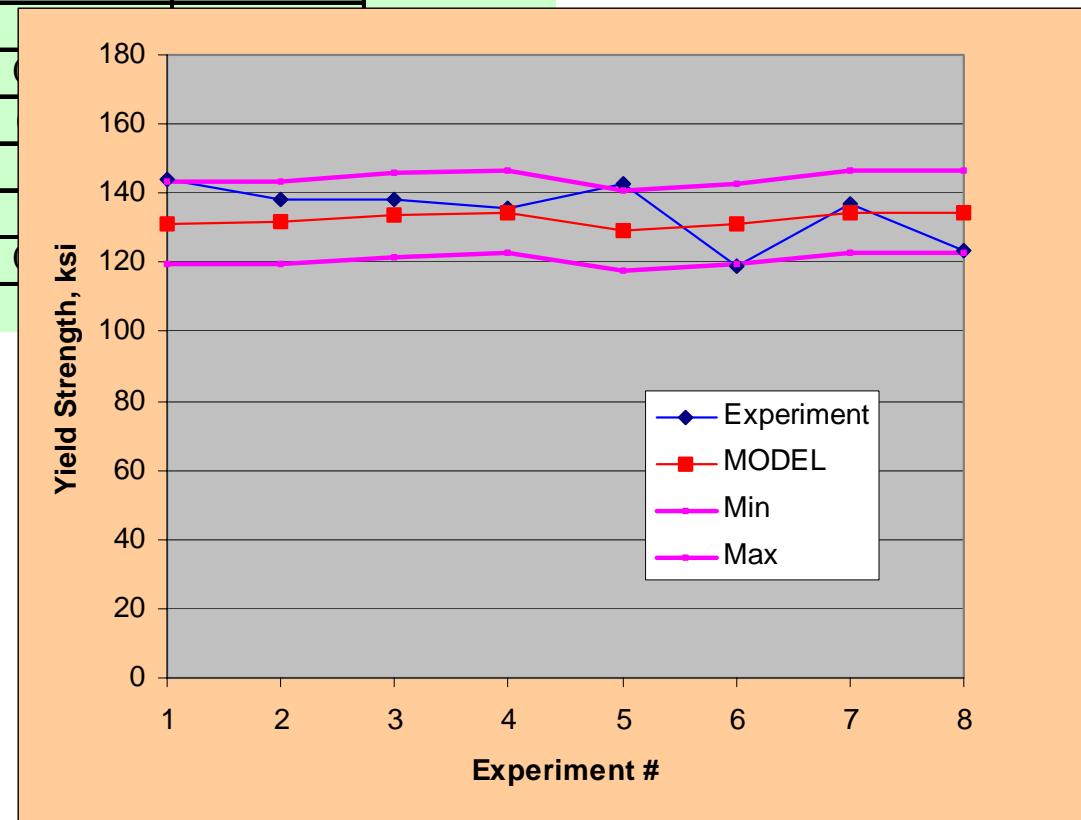


Rene 88 - 1200 F Data (from Pollock's slides)

Data from Pollock's slides

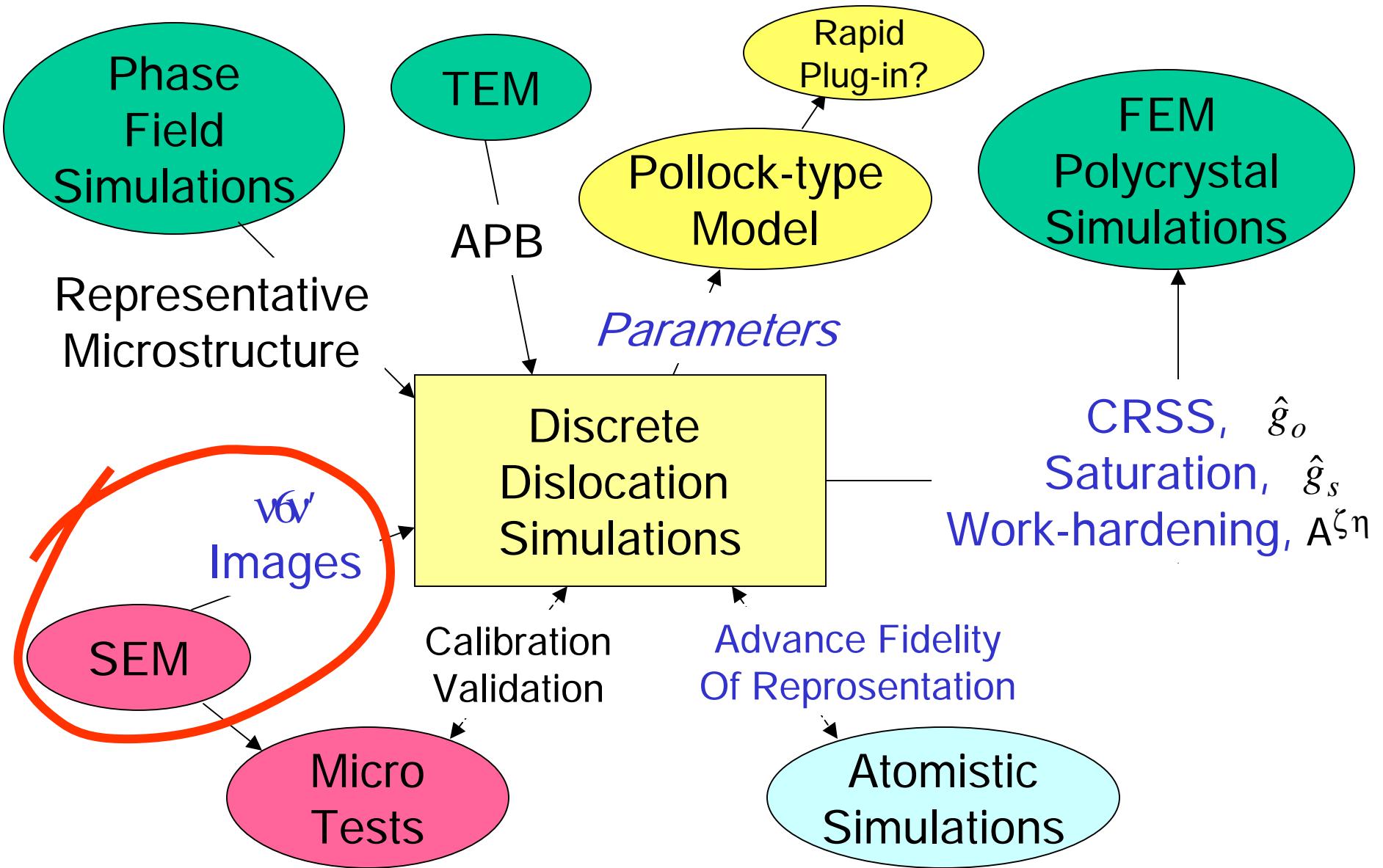
Clement / Nembach

Coh % 0.1	Experimental Data						$d_{(v2v')}$ 28.2	sol-g 33	sol-g' 200
	d_G' (um)	G' Fraction	d_G'' (um)	G'' Fraction	Yield Stress	YS (ksi)			
0.1478	0.2321	0.008474	0.1822	992.88	144				
0.1636	0.322	0.007317							
0.1489	0.32487	0.0393							
0.1669	0.3346	0.0153							
0.2738	0.1322	0.0083							
0.3865	0.2708	0.008							
0.2477	0.2416	0.017							
0.39	0.2771	0.0318							



APB	M	k_v
240	3	500

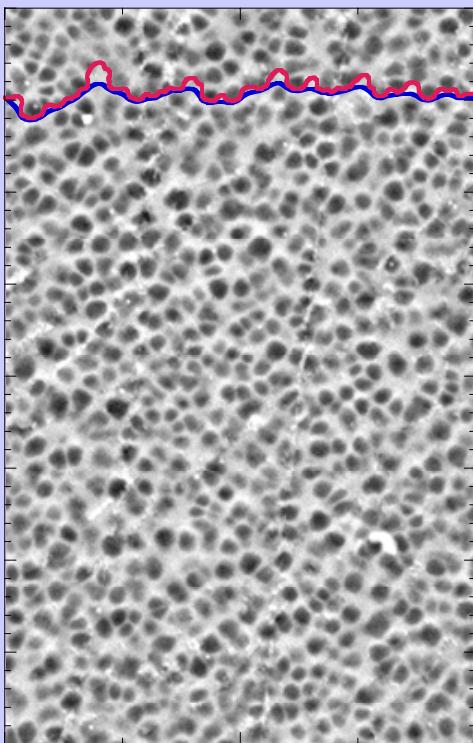
DD : Current Focus - Connectivity ("Handshakes")



SEM Image -> CRSS

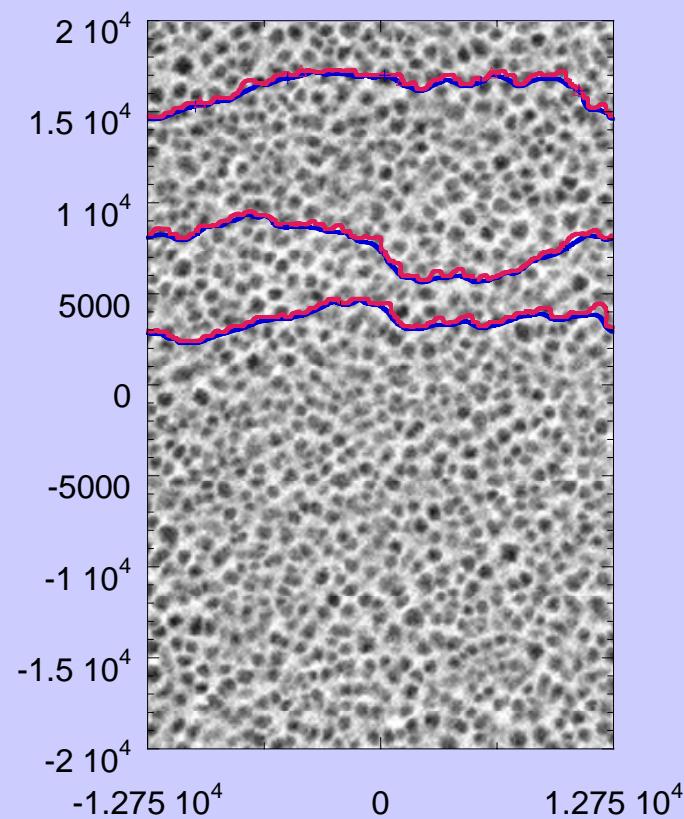
Bore

$\vartheta = 275 \text{ MPa}$



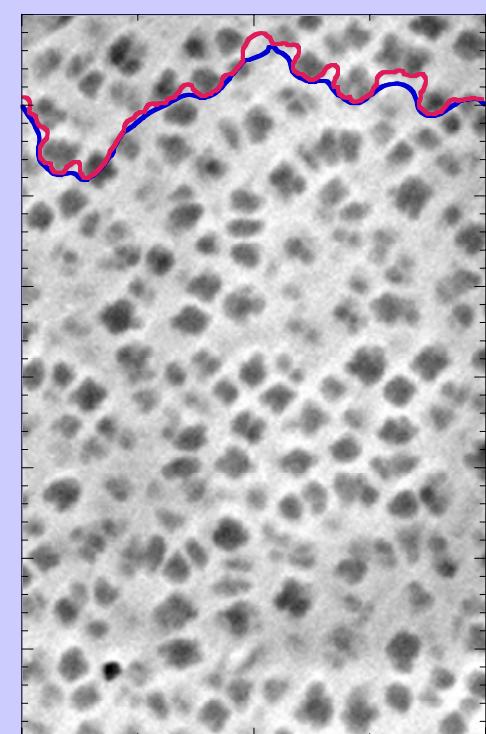
Rim

$\vartheta = 275 \text{ MPa}$

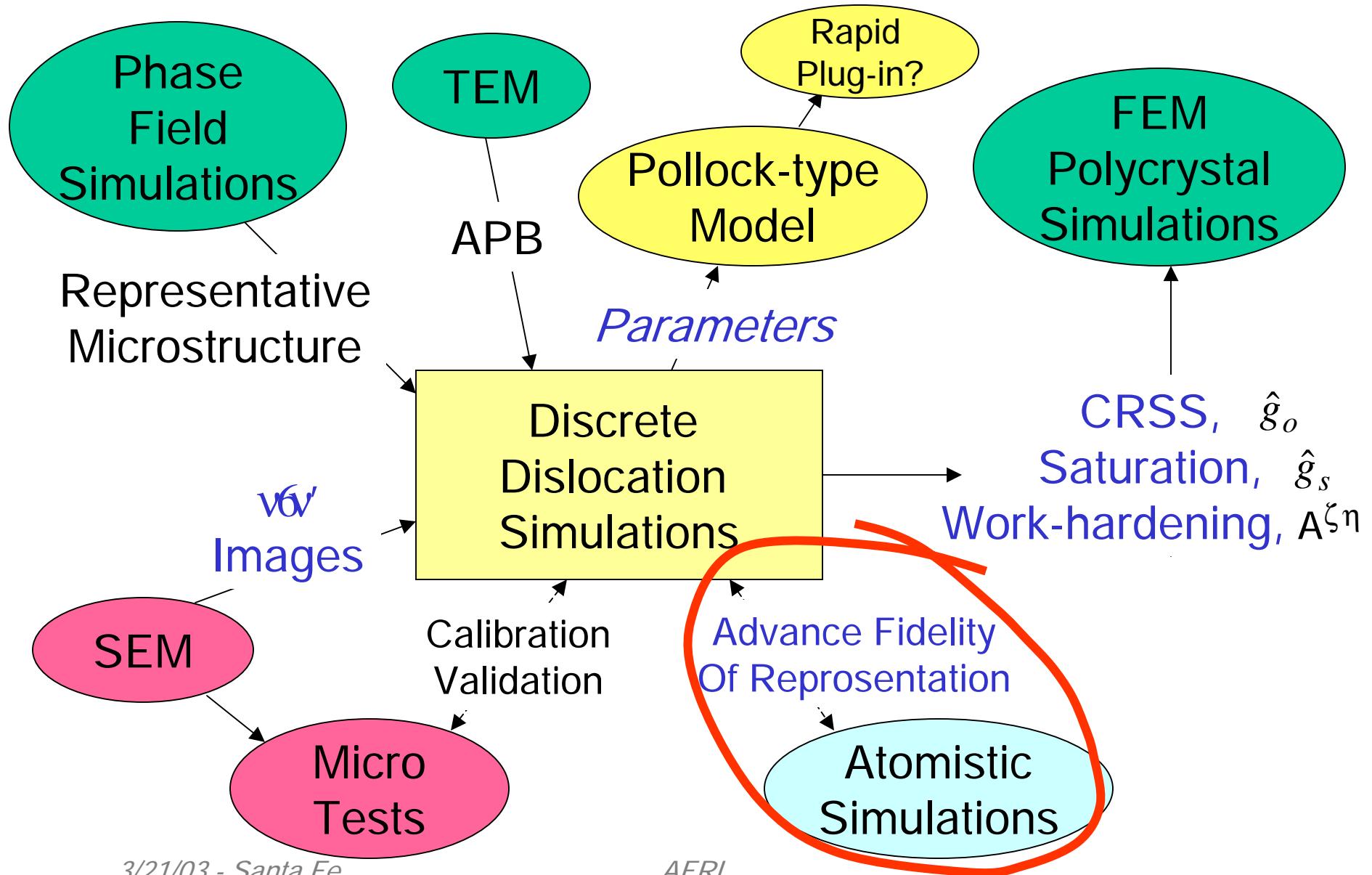


Web

$\vartheta = 265 \text{ MPa}$

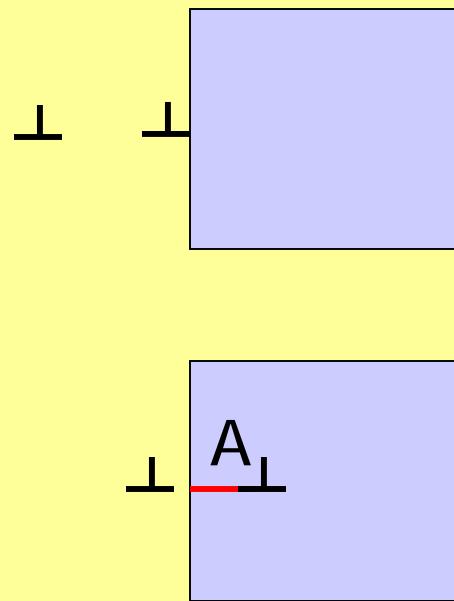


DD : Current Focus - Connectivity ("Handshakes")



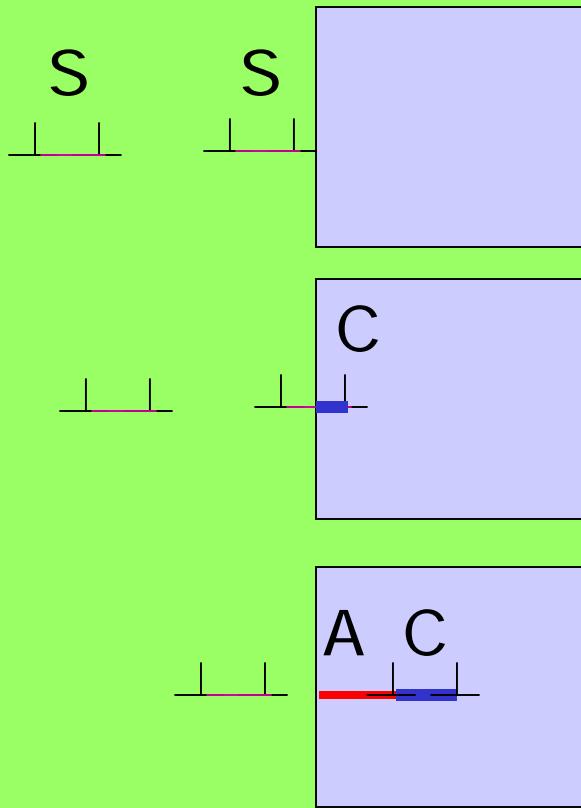
Atomistic Simulations -> Refinements of DD

DD Neglects Core Effects



*APB Energy
Critical Parameter*

Atomistics Include Core Effects



CSF, Core Effects Important ?
(Cross-slip within v')

Atomistics Simulation Validation Results

- EAM Potential with APB=140, CSF=120, SF(Ni)=60
- FLAT INTERFACE :

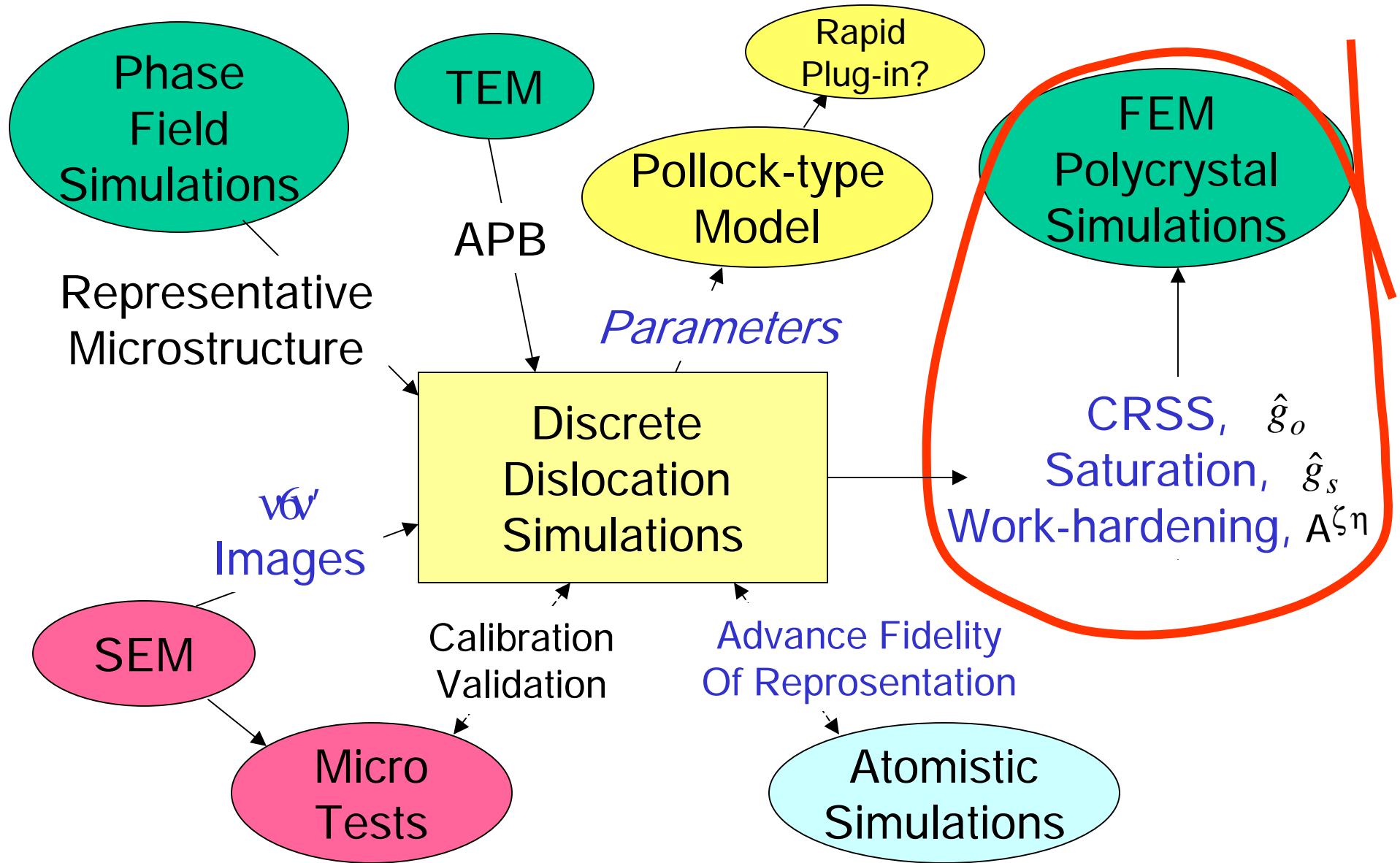
Atomistics

- Stress for first partial to enter : $(CSF-SF) / b$
- Stress for second partial to enter : $(APB) / b$
- No diffuse core effect

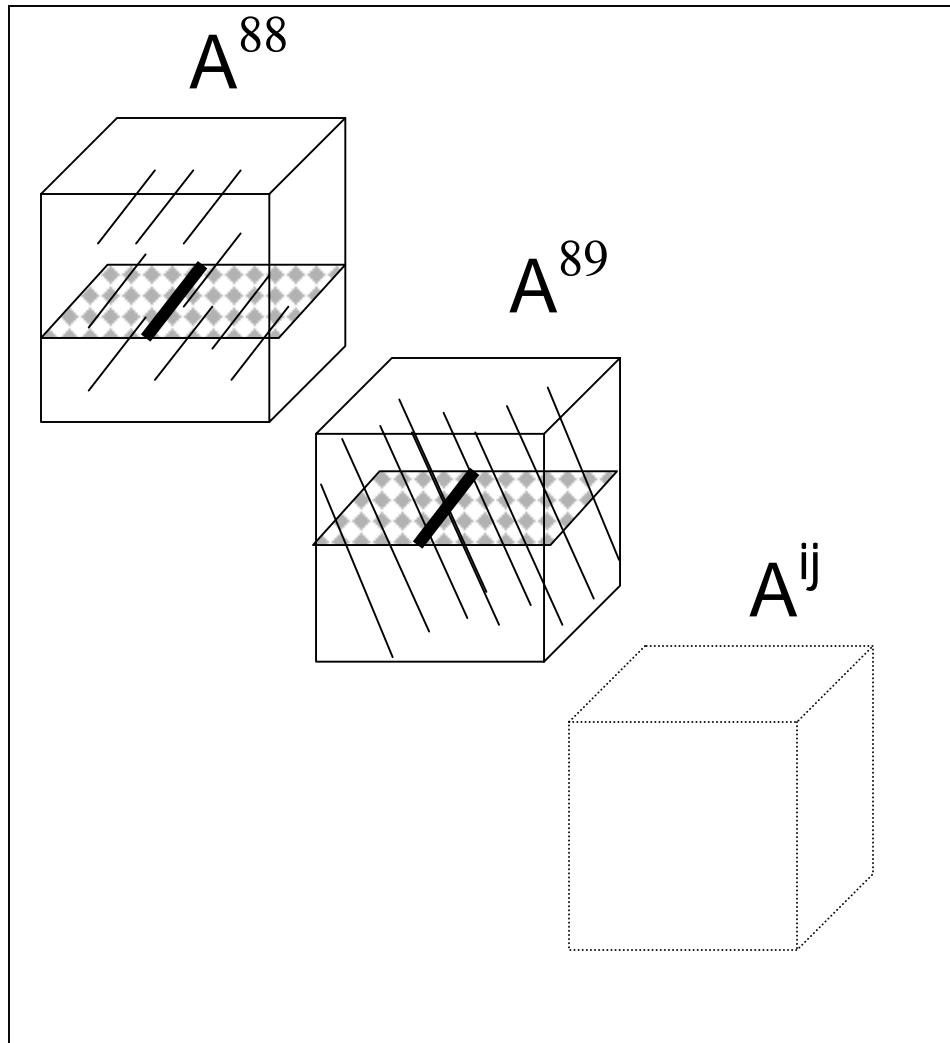
DD Max Stress = Stress for 1st DisIn entry = $(APB)/b$

=> APB Energy Sufficient , if APB $\geq (CSF-SF)$

DD : Current Focus - Connectivity ("Handshakes")

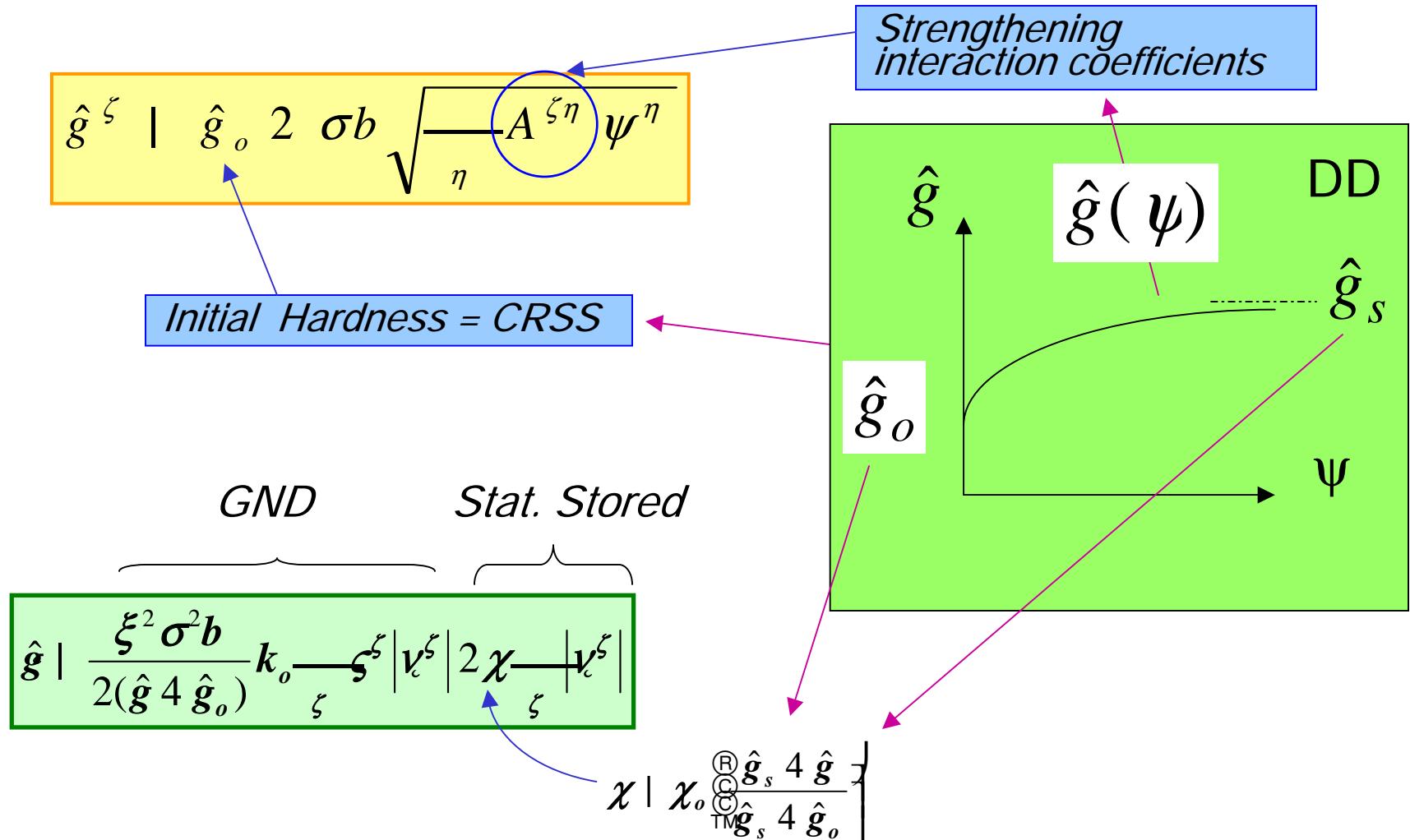


DD -> FEM Handoffs



DD -> FEM Handoffs

► γ Forest Obstacle Model (Franciosi, 1985)



OUTLINE

Microstructure Effects Within Grains ($v_2 v'$)

Using DD SIMULATIONS (S.Rao, T.A.Parthasarathy, D.M.Dimiduk, P.M.Hazzledine)

- PROGRESS : Established a Working Model / Methodology
- CURRENT FOCUS : Connectivity ("Handshakes")

Using FEM (Y-S Choi, T.A.Parthasarathy, D.M.Dimiduk)

- Unit Cell Model : Identified Key Issues - Refinements

Grain-Grain Interaction

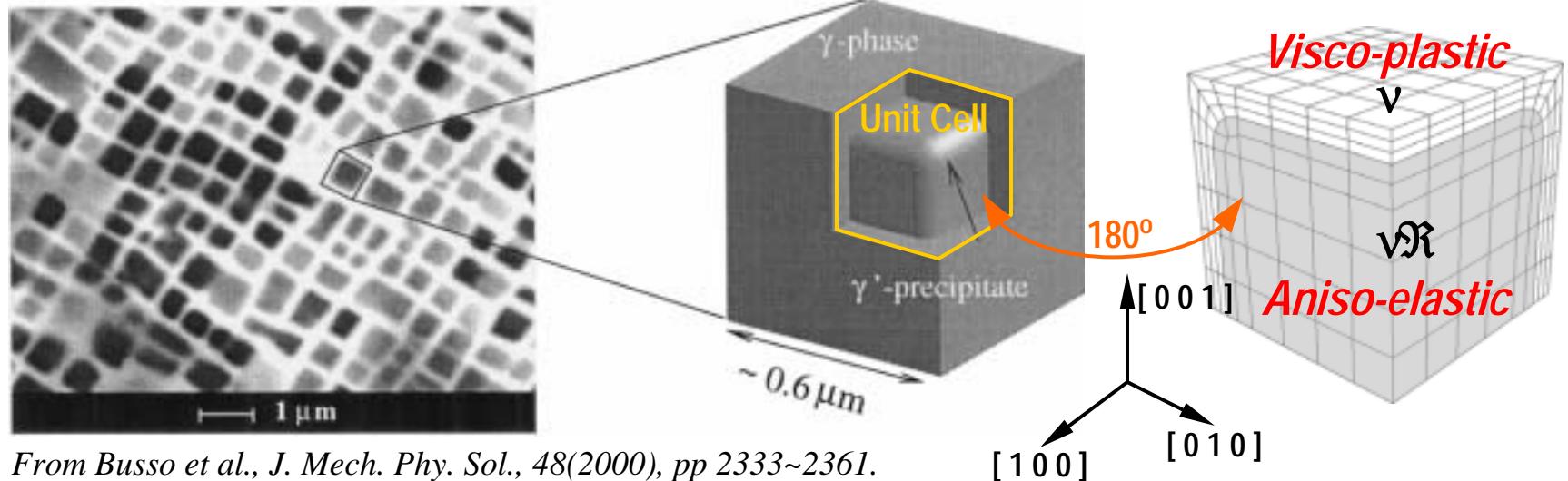
- Polycrystal Model : Using DD results

Grain-Defect Interaction

FEM : Unit Cell Model (Single Grain)

- Evaluated Unit Cell Approach using A-B Formalism
 - Yield Point -> determined by geometrical constraint
(different mechanism than DD)
 - W-H beyond Yield -> strain-gradient term dominant
- Refinement : Relaxation of Elastic ν' (using DD results)

FE Simulation of $(\nu+\nu')$: Unit Cell Approach



From Busso et al., J. Mech. Phys. Sol., 48(2000), pp 2333~2361.

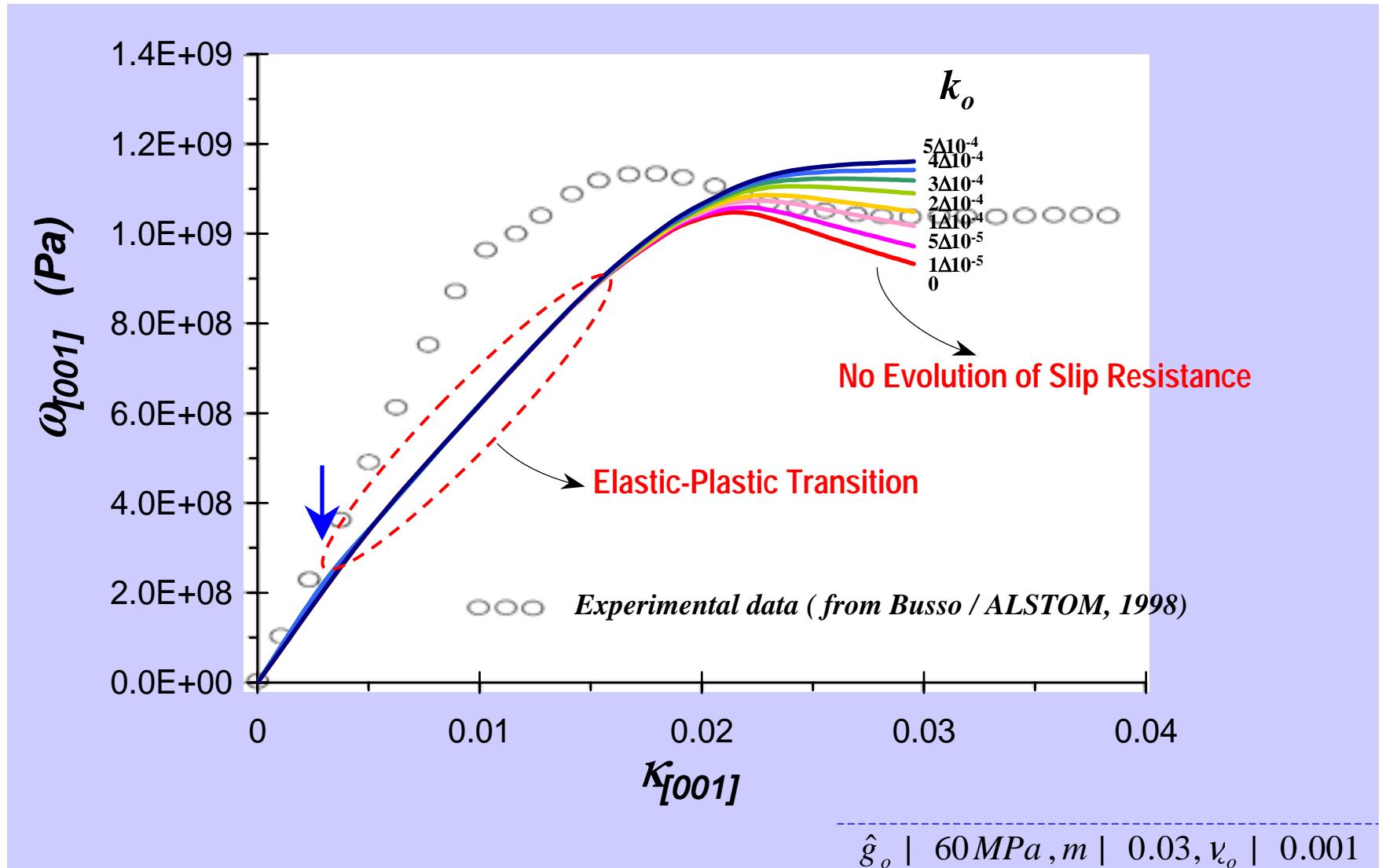
$$\nu^\zeta \mid \nu_o \operatorname{sgn}(\vartheta^\zeta) \left| \frac{\vartheta^\zeta}{\hat{g}^\zeta} \right|^{1/m}$$

with

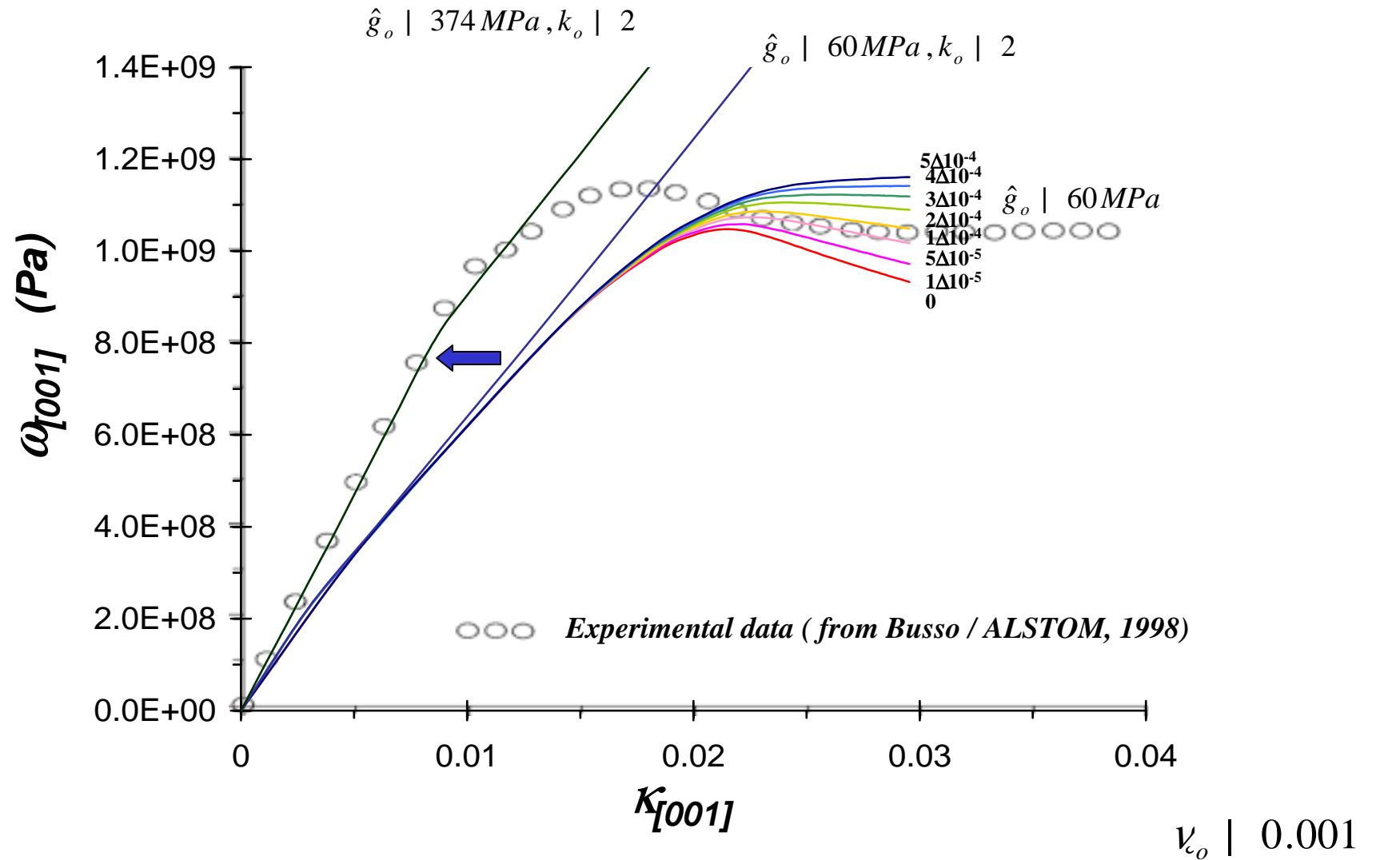
$$\hat{g}^\zeta \mid \frac{\xi^2 \sigma^2 b}{2(\hat{g} \cdot 4 \cdot \hat{g}_o)} k_o - \zeta \mid \nu^\zeta \mid$$

Only ζ^ζ (GND) contribution to slip resistance.

Effect of Strain-Gradient Parameter: k_o

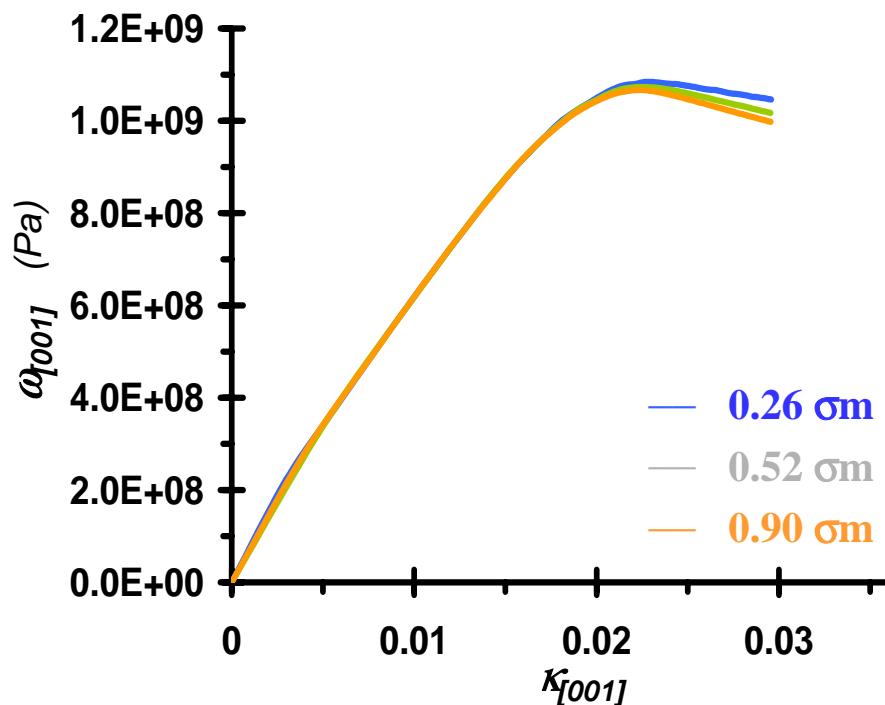


Effect of \hat{g}_o

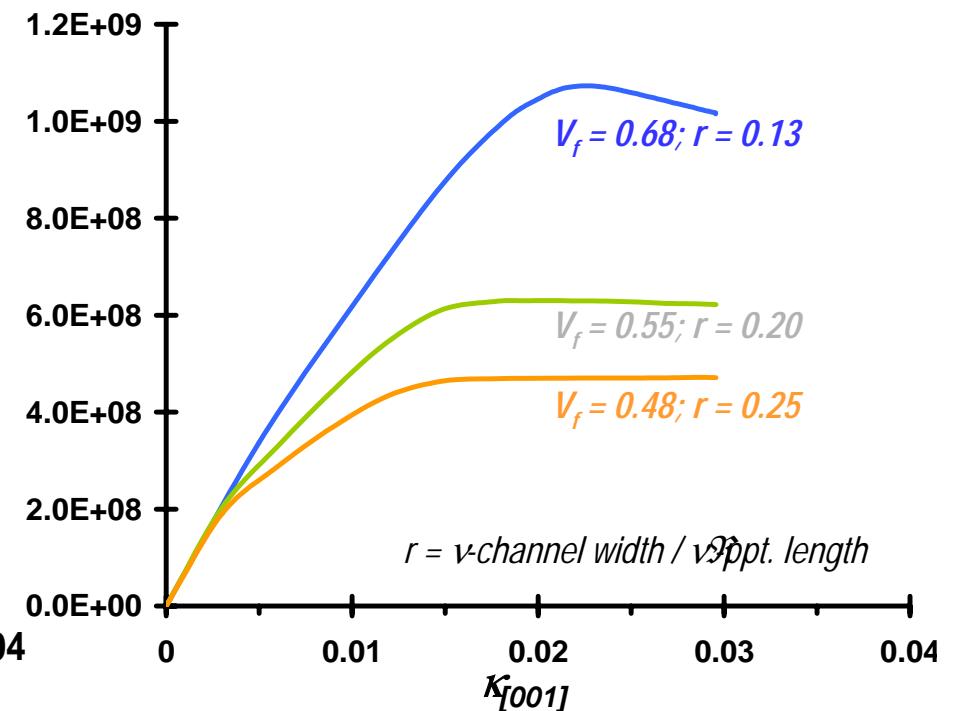


Length Scale Effects : ν Size, V_f

- ▶ Constant ν ppt. $V_f = 68\%$
- ▶ Change ν size (v-channel width)



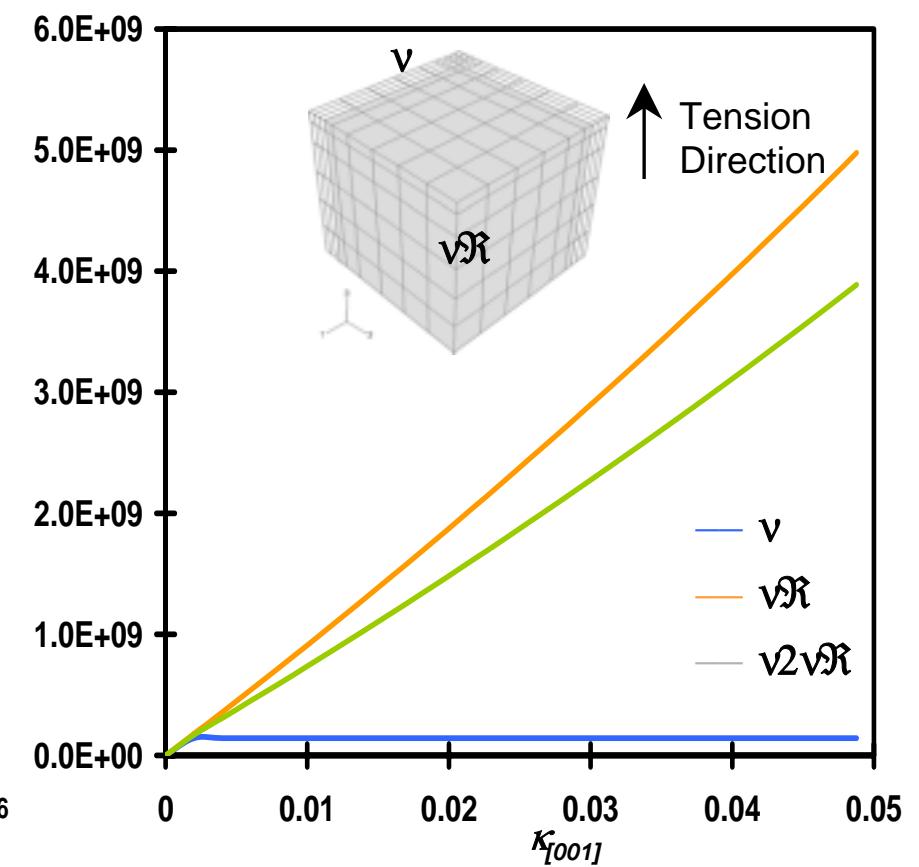
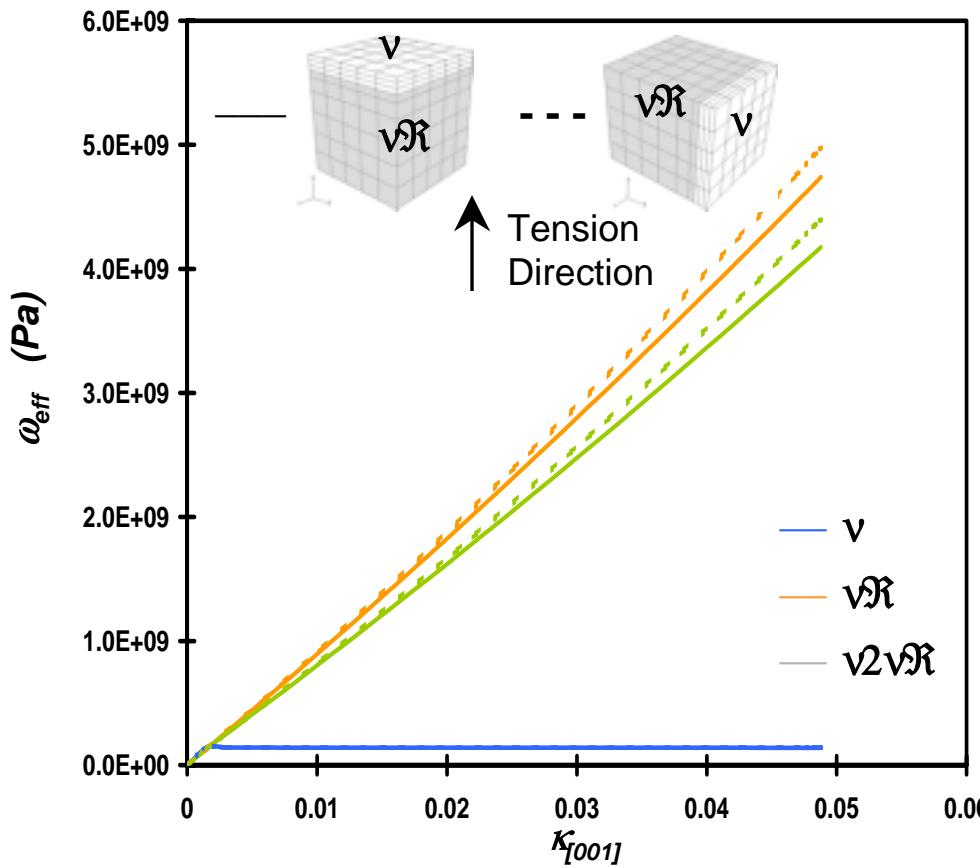
- ▶ Constant ν size = 0.52 σm
- ▶ Change ν V_f (v-channel width)



▶ $\hat{g}_o | 60 MPa, m | 0.03, \nu_o | 0.001, k_o | 5 \Delta 10^{45}$

Effect of $\nu/\sqrt{3}D$ Geometry

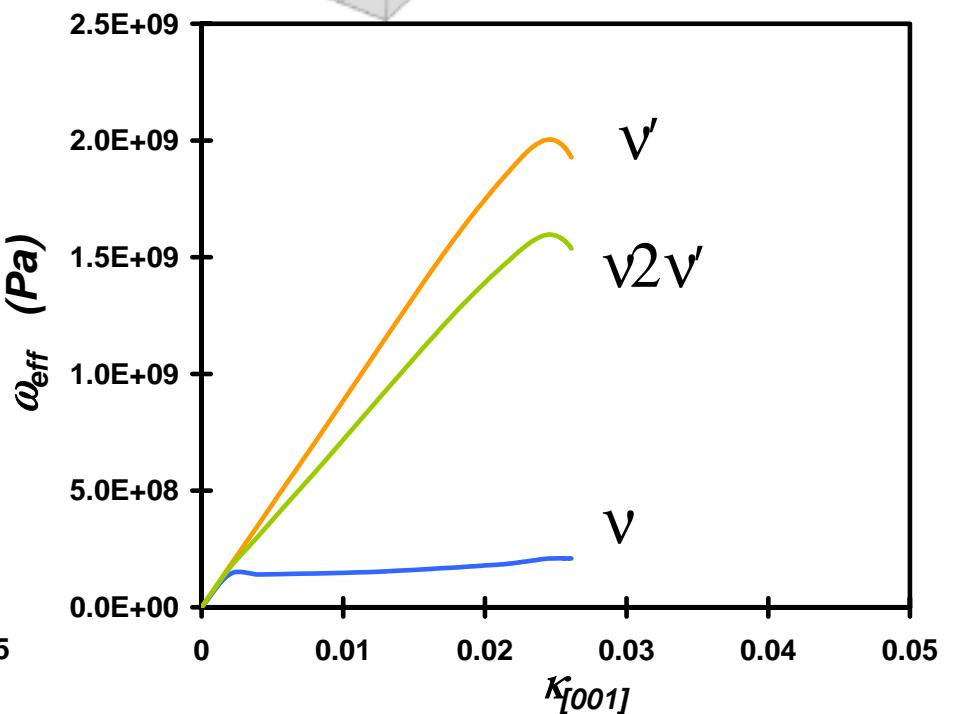
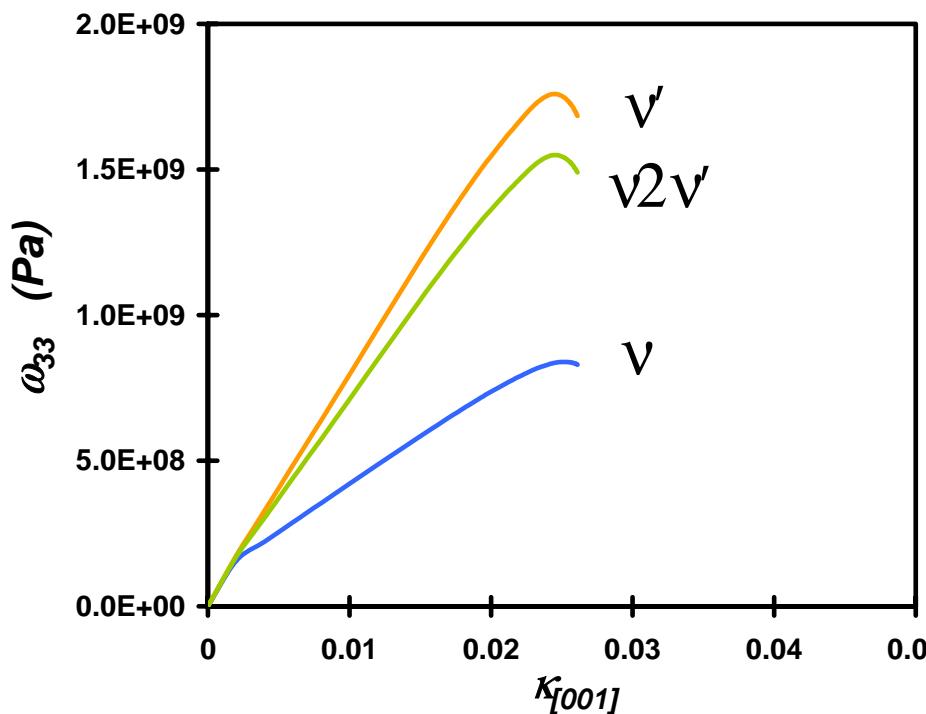
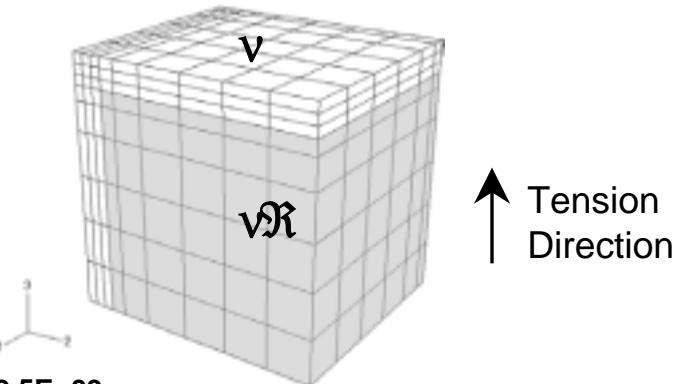
- ▶ Elastic ν Elasto-viscoplastic ν
- ▶ $\hat{g}_o \mid 60MPa, m \mid 0.03, \nu_o \mid 0.001, k_o \mid 0$ for Viscoplasticity

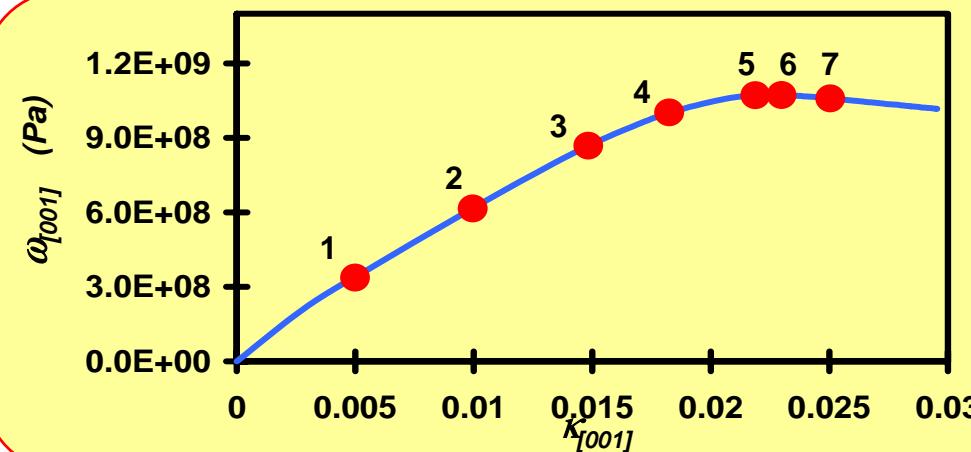


Effect of $\sqrt{V}R$ 3D Geometry

► Elastic \sqrt{V} Elasto-viscoplastic V'

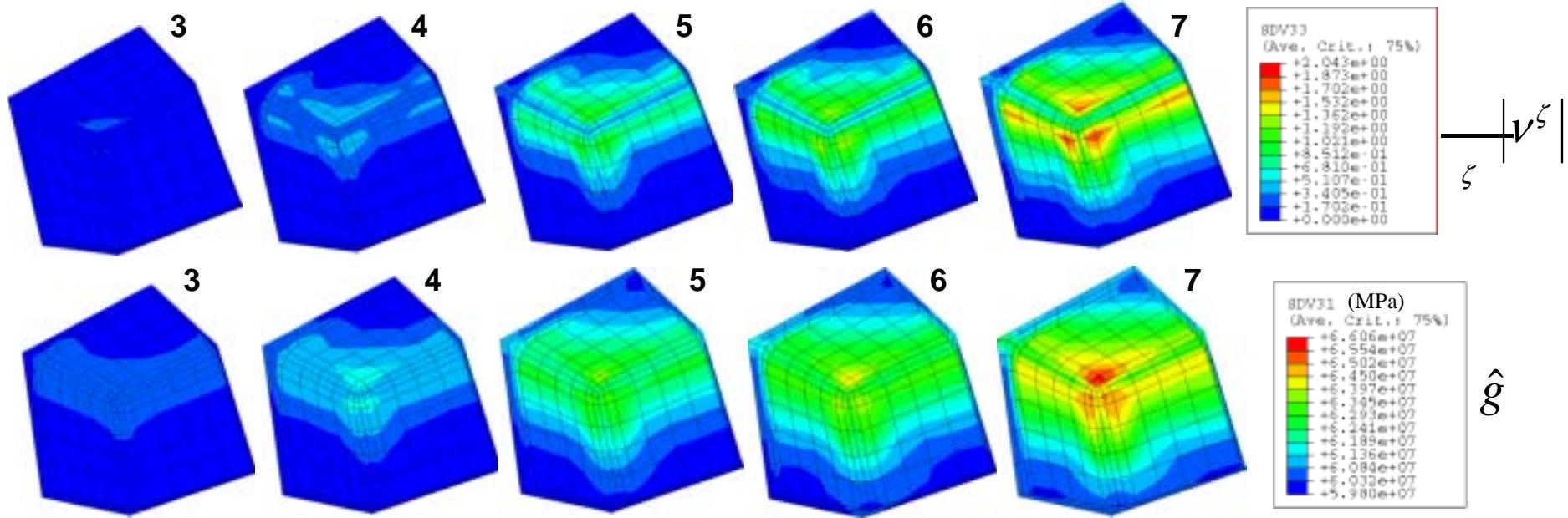
► $\hat{g}_o \mid 60MPa, m \mid 0.03, \nu_o \mid 0.001,$
 $k_o \mid 0$ for Viscoplasticity





V_f | 68%, ν_{size} | $0.52 \sigma_m$
 \hat{g}_o | 60 MPa , m | 0.03
 ν_o | 0.001, k_o | $5 \Delta 10^{45}$

[001]
[100]
[010]



- The onset of softening accompanied by the massive shears localized along the edges and the corners in the ν/ν interfaces
 - ♥ Break down of geometric (kinematic) constraints
 - ♥ Need to compare with experimental observations at this particular T-range

FEM : Unit Cell Model (Single Grain)

- Evaluated Unit Cell Approach using A-B Formalism
 - Yield Point -> determined by geometrical constraint
 - captures V_f Effect
 - W-H beyond Yield -> strain-gradient term dominant
 - captures size effect during work-hardening
- Refinement : Allow Plasticity in v' (using DD results)
 - DD captures APB cutting,
 - FEM captures Geometrical Constraint effect and Work Hardening

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Microstructure Effects Within Grains ($v_2 v'$)

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- Unit Cell Model : Identified Key Issues - Refinements

Grain-Grain Interaction

- Polycrystal Model : Using DD results

Grain-Defect Interaction

FEM : Polycrystal Model

- FY 2003 Goal : Combine DD with FEM to Build
1st gen. (v2v') Polycrystal model
 - Wigner-Seitz Cell (Beaudoin) - (144 grains, 12 el/gr)
 - Use DD results for g_o and A_{ij}
 - A-B model for Strain-gradient Terms
- Beyond FY2003
 - Build/Borrow v' const. Law to Model IN100 type alloy
 - Real Image 3D Polycrystal Models
 - Adaptive Meshing of Realistic Microstructures

Building Bridges : Inputs for Pollock-type Model

$$\omega_y / C_i, T, \kappa, \kappa, \dots 0 |$$

Needs Development Within Atomistics

$$f_v \frac{\textcircled{R} T_o}{\textcircled{T} M T} \left[\frac{dc}{\sqrt{dC_i}} \sqrt{C_i} \right] + M f_t \frac{\textcircled{R} B_{APB}}{\textcircled{T} M b}$$

Obtain by Dislocation Kinetics Simulation

$$+ \begin{cases} M \frac{4}{\phi^{1.5}} \frac{\int T_L}{bd_s} \sqrt{f/14} f_p 0 \sqrt{\frac{\textcircled{R} \phi d_s v}{2T_L} 4 1} & \text{strong coupling} \\ M \left(\frac{\textcircled{R} B}{\textcircled{T} M 2b} \right)^{1.5} \sqrt{\frac{2bd_s f/14 f_p 0}{T_L} \frac{\int 4}{\phi^{1.5}} 4 \frac{Bf/14 f_p 0}{2b}} & \text{weak coupling} \end{cases}$$

Obtain by FEM Simulation of Grain Distribution Effects

$$+ /14 f_p k_y^v \frac{1}{\sqrt{d_v}} + f_p \left(\omega/T 0_{Ni_3Al} 2 - \frac{\textcircled{R} dc}{\textcircled{T} M dC_i} C_i \right) + f_p k_y^v \frac{1}{\sqrt{d_{vR}}}$$

Building Bridges

TO

- Inputs for Pollock-type Model 3-6 mo.
- Fatigue Models (McDowell,...) 1-2 yrs

FROM

- v' Constitutive Laws (Parks, Cuitino/Ortiz, ...) 3-6 mo.
- 3D Voronoi Meshing (Parks, Gosh, ..) 3-6 mo.